

Analysis of Electronic and Structural Properties of Surfaces and Interfaces Based on LaAlO₃ and SrTiO₃

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Abstract

© 2016, Springer Science+Business Media New York. Recently, it was established that a two-dimensional electron system can arise at the interface between two oxide insulators LaAlO₃ and SrTiO₃. This paradigmatic example exhibits metallic behaviors and magnetic properties between non-magnetic and insulating oxides. Despite a huge amount of theoretical and experimental work a thorough understanding is yet to be achieved. We analyzed the structural deformations of a LaAlO₃ (001) slab induced by hydrogen adatoms and oxygen vacancies at its surface by means of density functional theory. Moreover, we investigated the influence of surface reconstruction on the density of states and determined the change of the local density of states at the Fermi level with increasing distance from the surface for bare LaAlO₃ and for a conducting LaAlO₃/SrTiO₃ interface. In addition, the Al-atom displacements and distortions of the TiO₆-octahedra were estimated.

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Keywords

Defects, Density functional, Electronic structure, Interface, LAO/STO, Surface